

Nitromethane
75-52-5 | DTXSID2020977

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 9.41e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.41e-01

Confidence level: 6.99e-01

Nearest Neighbors from the Training Set

Image not found

Nitromethane

Measured: 1.82

Predicted: 9.41e-01

Image not found

Nitroethane

Measured: 6.26e-01

Predicted: 4.35e-01

Image not found

1-Nitropropane

Measured: 1.68e-01

Predicted: 2.14e-01

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2-Nitropropane

Measured: 2.15e-01

Predicted: 2.16e-01